

## CLAIMS

What is claimed as new and desired to be protected by Letters Patent of the United States is:

5 1. A system for integrated modeling, simulation and analysis of a biological system that includes processes that may be described by chemical reactions, the system comprising:

a modeling component for constructing a model of the biological system;

10 a simulation engine in communication with said modeling component, said simulation engine accepting as input the constructed model of the biological system and generating dynamic behavior of the constructed model as output; and

an analysis environment in communication with said simulation engine and said modeling component, said analysis environment for analyzing aspects of the constructed model.

15 2. The system of claim 1 wherein the modeling component comprises an environment for construction of a block diagram model of the biological system.

3. The system of claim 2 wherein the modeling component further includes at least one block identifying a set of related chemical reactions.

4. The system of claim 1 wherein the modeling component accepts user commands and input for constructing the model of the biological system.

20 5. The system of claim 1 wherein said simulation engine generates the dynamic behavior of the constructed model using a stochastic computational model.

6. The system of claim 1 wherein said simulation engine generates the dynamic behavior of the constructed model using a discrete time-based computational model.

25 7. The system of claim 1 wherein said simulation engine generates the dynamic behavior of the constructed model using a continuous time-based computational model.

8. A method for integrated modeling, simulation and analysis of a biological process comprising a plurality of chemical reactions, the method comprising the steps of:

- (a) constructing a model of a the biological process;
- (b) generating, using the constructed model of the biological process,  
dynamic behavior of the modeled biological process; and
- (c) displaying the dynamic behavior on a display device.

9. The method of claim 8 wherein step (a) comprises constructing a block diagram model of a chemical reaction that is part of the biological process.

10. The method of claim 9 wherein the block diagram model includes at least one block identifying a set of related chemical reactions that are part of the biological process.

11. The method of claim 8 where step (a) further comprises:

- (i) providing a graphical user interface for accepting user commands and data;
- (ii) receiving, via the provided graphical user interface, user commands and data; and
- (iii) constructing, using the received user commands and data, a model of the biological process.

12. The method of claim 8 wherein step (b) comprises generating, using the constructed model of the biological process, dynamic behavior of the modeled biological process using a stochastic computational model.

13. The method of claim 8 wherein step (b) comprises generating, using the constructed model of the biological process, dynamic behavior of the modeled biological process using a discrete time-based computational model.

14. The method of claim 8 wherein step (b) comprises generating, using the constructed model of the biological process, and dynamic behavior of the modeled biological process using a continuous time-based computational model.

15. An article of manufacture having embodied thereon computer-readable program means for integrated modeling, simulation and analysis of biological processes, the article of manufacture comprising:

5 computer-readable program means for constructing a model of a biological process;

computer-readable program means for generating, using the constructed model of the biological process, an expected output of the modeled biological process; and

computer-readable program means for displaying the dynamic behavior.

10 16. The article of manufacture of claim 15 wherein said computer-readable program means for constructing a model of the biological process comprises computer-readable program means for constructing a block diagram model of a biological process.

15 17. The article of manufacture of claim 16 wherein said computer-readable program means for constructing a block diagram model of the biological process includes computer-readable program means for constructing at least one block identifying a set of related chemical reactions.

20 18. The article of manufacture of claim 15 wherein computer-readable program means for generating an dynamic behavior of the modeled biological process comprises computer-readable program means for generating an expected result of the modeled biological process using a stochastic computational model.

19. The article of manufacture of claim 15 wherein computer-readable program means for generating an dynamic behavior of the modeled biological process comprises computer-readable program means for generating an expected result of the modeled biological process using an event-based computational model.

25 20. A method for integrated modeling, simulation and analysis of a biological process comprising a plurality of chemical reactions, the method comprising the steps of:

(a) constructing a model of a biochemical process in a modeling component;

(b) analyzing the constructed model of the biological process to generate a result; and

(c) transmitting the result to the modeling component.

21. The method of claim 20 wherein step (b) comprises analyzing the constructed model of the biological process using bifurcation analysis.

22. The method of claim 20 wherein step (b) comprises analyzing the constructed model of the biological process using sensitivity analysis.

23. The method of claim 20 where step (b) comprises analyzing the constructed model of the biological process using parameter estimation.

24. The method of claim 20 wherein step (b) comprises analyzing the constructed model of the biological process using a non-linear solver.

25. The method of claim 20 wherein step (b) comprises analyzing the constructed model of the biological process using flux-balance analysis.

26. A system for integrated modeling, simulation and analysis of a chemical reaction comprising:

a modeling component for constructing a model of the chemical reaction;

a simulation engine in communication with said modeling component, said simulation engine accepting as input the constructed model of the chemical reaction and generating an expected output based on the model; and

an analysis environment in communication with said simulation engine and with said modeling component, said analysis environment performs analysis and displays the expected output.

27. The system of claim 26 wherein the modeling component comprises an environment for construction of a block diagram model of a chemical reaction.

28. The system of claim 27 wherein the modeling component further includes at least one block identifying a set of related chemical reactions.

29. The system of claim 26 wherein the modeling component accepts user commands and input for constructing the model of the chemical reaction.

30. The system of claim 26 wherein said simulation engine generates the expected output using a stochastic computational model.

5 31. The system of claim 26 wherein said simulation engine generates the expected output using a discrete time-based computational model.

32. The system of claim 26 wherein said simulation engine generates the expected output using a continuous time-based computational model.

10 33. A method for integrated modeling, simulation and analysis of chemical reactions, the method comprising the steps of:

(a) constructing a model of a chemical reaction;

(b) generating, using the constructed model of the chemical reaction, an expected output of the modeled chemical reaction; and

(c) displaying the expected output on a display device.

15 34. The method of claim 33 wherein step (a) comprises constructing a block diagram model of a chemical reaction.

35. The method of claim 34 wherein the block diagram model includes at least one block identifying a set of related chemical reactions.

36. The method of claim 33 wherein step (a) comprises:

20 (i) providing a graphical user interface for accepting user commands and data;

(ii) receiving, via the provided user interface, user commands and data; and

25 (iii) constructing, using the received user commands and data, a model of the chemical reaction.

37. The method of claim 33 wherein step (b) comprises generating, using the constructed model of the chemical reaction, an expected output of the modeled chemical reaction using a stochastic computational model.

5 38. The method of claim 33 wherein step (b) comprises generating, using the constructed model of the chemical reaction, an expected output of the modeled chemical reaction using a discrete time-based computational model.

39. The method of claim 33 wherein step (b) comprises generating, using the constructed model of the chemical reaction, an expected output of the modeled chemical reaction using a continuous time-based computational model.

10 40. An article of manufacture having embodied thereon computer-readable program means for integrated modeling, simulation and analysis of chemical reactions, the article of manufacture comprising:

computer-readable program means for constructing a model of a chemical reaction;

15 computer-readable program means for generating, using the constructed model of the chemical reaction, an expected output of the modeled chemical reaction; and

computer-readable program means for displaying the expected output.

20 41. The article of manufacture of claim 40 wherein said computer-readable program means for constructing a model of the chemical reaction comprises computer-readable program means for constructing a block diagram model of a chemical reaction.

25 42. The article of manufacture of claim 41 wherein said computer-readable program means for constructing a block diagram model of the chemical reaction includes computer-readable program means for constructing at least one block identifying a set of related chemical reactions.

43. The article of manufacture of claim 40 wherein computer-readable program means for generating an expected result of the modeled chemical reaction comprises

computer-readable program means for generating an expected result of the modeled chemical reaction using a stochastic computational model.

44. The article of manufacture of claim 40 wherein computer-readable program means for generating an expected result of the modeled chemical reaction comprises computer-readable program means for generating an expected result of the modeled chemical reaction using an event-based computational model.

45. A method for integrated modeling, simulation and analysis of chemical reactions, the method comprising the steps of:

- (a) constructing a model of a chemical reaction;
- (b) analyzing the constructed model of the chemical reaction to generate a result; and
- (c) transmitting the result to the modeling environment.

46. The method of claim 45 wherein step (b) comprises analyzing the constructed model of the chemical reaction using bifurcation analysis.

47. The method of claim 45 wherein step (b) comprises analyzing the constructed model of the chemical reaction using sensitivity analysis.

48. The method of claim 45 wherein step (b) comprises analyzing the constructed model of the chemical reaction using parameter estimation.

49. The method of claim 45 wherein step (b) comprises analyzing the constructed model of the chemical reaction using a non-linear solver.

50. The method of claim 45 wherein step (b) comprises analyzing the constructed model of the chemical reaction using flux-balance analysis.

51. The method of claim 45 wherein step (b) comprises generating, using the constructed model of the chemical reaction, an expected result of the modeled chemical reaction using a continuous time-based computational model.